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COLLECTIVE MOTION AND THE GENERATOR COORDINATE METHOD

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E.J.V. de Passos*

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The generator coordinate method is used to construct a collective subspace of the many-body Hilbert space. The construction is based on the analysis of the properties of the overlaps of the generator states. Some well-known misbehaviours of the generator coordinate weight functions are clearly identified as of kinematical origin. A standard orthonormal representation in the collective subspace is introduced which eliminates them. It is also indicated how appropriate collective dynamical variables can be defined a posteriori. To illustrate the properties of the collective subspaces applications are made to

a) translational invariant overlap kernels

b) to one and two-conjugate parameter families of generator states.

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I - THE KINEMATICS OF GENERATOR COORDINATES

In the generator coordinate method (GCM) there is a clear separation of two stages in the setting up of a phenomenological scheme to describe collective motion of many-body systems.

In the first stage we select a subspace of the many-body Hilbert space (HS) which is spanned by states constructed as a linear superposition of the generator states $|\alpha\rangle^{(1)}$.

 $\mathbf{f}_{\mathbf{z}}^{\dagger} \neq = \int_{-\infty}^{+\infty} \mathbf{f}(\alpha) |\alpha|^{2} \frac{d\alpha}{d\alpha} d\alpha = \mathbf{g}(\alpha) \mathbf{g}($

with square integrable weight function $f(\alpha)$.

The generator states $|\alpha\rangle$ are specified a priori usually on the basis of phenomenological considerations in a way to reflect the distortion of the many-body system during the collective motion. The parameter α is the generator coordinate and it establishes a one to one mapping between the generator states and points in a label space.

In contrast to other approaches $^{(1)}$, which use product type wave functions, the GCM does not require an explicit reference to any collective dynamical variable at this stage. Indeed, the specification of the appropriate collective degrees of freedom is in general very difficult, the adequacy of a given choice being a dynamical question which cannot be settled without explicit reference to the many-body hamiltonian. Furthermore even in the cases when one has a good phenomenological knowledge as to the nature of the collective motion under consideration it is, in general, very difficult to find an explicit expression for the collective degrees of freedom in terms of the microscopic ones $^{(1)}$. These desadvantages are absent in the GCM.

The dynamics is established in the second stage with the determination of the weight function $f(\alpha)$, the only unknown in eq. I.1.

The states given by the ansatz I.l are used as trial wave functions in the variational principle

$$\frac{\langle \mathbf{f} | \mathbf{H} | \mathbf{f} \rangle}{\langle \mathbf{f} | \mathbf{f} \rangle} \stackrel{\text{resc}}{=} 0^{1/2} \quad \text{for a rescale of the second states of the s$$

resulting in the Griffin-Hill-Wheeler (GHW) integral equation for f(α) ⁽¹⁾

$$\int (\langle \alpha | H | \alpha' \rangle - E \langle \alpha | \alpha' \rangle) f(\alpha') d\alpha' = 0$$

2

I.2

The GCM is probably less a accurate than methods involving the explicit introduction of collective dynamical variables ⁽¹⁾ in cases for which this explicit introduction is straightforward. Unfortunately this is not the case in general and the GCM provides a scheme which is very easy to apply in practice ⁽²⁾. However in this lecture I would like to discuss the GCM description of collective dynamics with especial emphasis on questions of interpretation. To do so, the first difficult that one has to face is the well known fact that, in many cases, the weight functions $f(\alpha)$ have undesirable mathematical properties ⁽³⁾. The consequence of this fact is that the GHW ansatz (I.1) will associate highly singular weight functions to vectors defined in the many-body H.S..

This difficulty can be shown to be simply a consequence of the use of the non-orthogonal and, in general, linearly dependent generator states $|\alpha\rangle$ as a representation in the GCM collective subspace S and it is eliminated by introducing a standard orthonormal representation in S. This standard orthonormal representation is constructed in terms of the adopted set of generator states and it allow us to define, a posteriori, the collective hamiltonian, collective dynamical variables and collective wave functions.

The basic tool of the method is the diagonalization of the overlap kernel <a $|\alpha|$ > ^(4,5,6)

 $\int_{-\infty}^{+\infty} <\alpha \, | \, \alpha' > u_{\mathbf{k}}(\alpha') \, d\alpha' = \Lambda(\mathbf{k}) u_{\mathbf{k}}(\alpha)$ are real rate to be reach the rate of \mathbf{L} . So the

The eigenfunctions of the overlap kernel form an orthogonal and complete set

$$\int_{-\infty}^{+\infty} u_{\mathbf{k}}^{*} (\alpha) u_{\mathbf{k}}^{*} (\alpha) d\alpha = \delta (\mathbf{k} - \mathbf{k}^{*})$$

$$\int_{-\infty}^{+\infty} u_{\mathbf{k}}^{*} (\alpha) u_{\mathbf{k}}^{*} (\alpha^{*}) d\mathbf{k} = \delta (\alpha - \alpha^{*})$$
I.4

In eq. I.3, $\Lambda(k)$ is always a semi-positive definite function of k (the overlap kernel is a norm) and for simplicity it will be assumed to be a monotonic decreasing function of k vanishing only at $|k| \not\rightarrow \infty$. The general case is discussed in ref. 6. To proceed we need to be specific and we define the <u>GHW space</u> as the space spanned by the many-body vectors constructed as in I.1 with square integrable weight functions. The scalar product of two such vectors is equal to

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4

Therefore to each vector defined in the GHW space we can associate a square integrable function $\tilde{f}(k)$, which is equal to the scalar product of $|f\rangle$ with the orthogonal state $|k\rangle$. However the inverse is not true. To show this we write the weight function as

 $f(\alpha) = \int dk \ u_k(\alpha) \ \frac{\tilde{f}(k)}{\sqrt{\Lambda(k)}}$ I.8

Thus $f(\alpha)$ is a regular function only if $f(k)/\sqrt{h(k)}$ goes to zero when |k| goes to infinite. Otherwise it is singular. At this point we consider the extension of the GHW space to a subspace of the many-body H.S. in which the vectors have square integrable $\tilde{f}(k)$. This extended space is the GCM collective subspace S and the projection operator in S is given by

 $\hat{\mathbf{S}} = \int d\mathbf{k} |\mathbf{k} > \langle \mathbf{k} |$

From the previous discussion it is clear that not all vectors defined in the GCM collective subspace S belongs to the GHW space. However it can be shown⁽⁵⁾ that the GHW space is dense in S and the subspace S is the smallest (closed) subspace which contains the G.H.W space. Therefore we can say that the singular behaviour of the weight function is related to the fact that strictly speaking, the generator state is a well-behaved representation of the GHW space but not of the GCM collective subspace.

II - DYNAMICS IN THE GCM COLLECTIVE SUBSPACE - COLLECTIVE HAMILTONIAN, COLLECTIVE OPERATORS AND COLLECTIVE WAVE-FUNCTIONS

The description of the dynamics in the GCM is given by the projection of the many-body dynamics onto the collective subspace S

$$i \partial_{t} |\psi(t)\rangle = \hat{H}_{c}^{GCM} |\psi(t)\rangle$$

where

$$\hat{S} | \psi(t) \rangle = | \psi(t) \rangle$$

In eq. II.1 $\underline{\hat{H}}_{C}^{CCM}$ is the GCM collective hamiltonian. It is the projection of the many-body hamiltonian onto the GCM collective subspace S,

$$\hat{H}_{C}^{GCM} = \hat{S} \hat{H} \hat{S}$$
 II.2

Using the expression I.9 of the projection operator S, we can write the dynamical equation II.1 as a wave-equation in the "momentum" representation $|k\rangle$

$$\int h(k,k') \phi(k',t) dk' = i \frac{\partial \phi(k,t)}{\partial t}$$
 II.3

where

$$h(\mathbf{k},\mathbf{k}^{\dagger}) = \langle \mathbf{k} | \hat{\mathbf{H}} | \mathbf{k}^{\dagger} \rangle$$

$$= \int d\alpha d\alpha^{\dagger} \frac{\mathbf{u}_{\mathbf{k}}^{\star}(\alpha) \langle \alpha | \hat{\mathbf{H}} | \alpha^{\dagger} \rangle - \mathbf{u}_{\mathbf{k}^{\dagger}}(\alpha^{\dagger})}{\sqrt{\Lambda(\mathbf{k})}} \qquad \text{II.4}$$

and $\phi(k,t)$ is the collective wave-function in the "momentum" representation

$$\phi(\mathbf{k},\mathbf{t}) = \langle \mathbf{k} | \phi(\mathbf{t}) \rangle^{1/2} \qquad \text{II.5}$$

ÏI.1

The above discussion was carried in the specific representation that diagonalizes the overlap kernel. Although this representation is very convenient for sorting out the kinematical oddities inherent to the GCM, other representations may be prefereable from a physical point of view. They can be obtained by unitary transformations in S. One which has been considered often in the literature (1,7,8) is the "coordinate" representation obtained by an unitary transformation of the "momentum" representation given in terms of the eigenfunctions of the overlap kernel $\langle \alpha | \alpha \rangle$

 $\|\eta\rangle = \int_{-\infty}^{+\infty} |k\rangle |u_k^*(\eta) \frac{dk}{dk} = \frac{1}{2} \int_{-\infty}^{+\infty} |u|^$

As pointed out before, in the GCM there is no explicit reference to any collective dynamical variable. However once one has a representation in the collective subspace, one can define, à posteriori, collective dynamical variables in S. These collective dynamical variables would allow us to describe the dynamics in terms of a small number of specialized degrees of freedom. As an example $\binom{9}{}$ we can associate to the coordinate representation II.6, a pair of canonical operators in S,

 $\hat{Q}_{\eta} | \eta \rangle = \eta | \eta \rangle$ $\hat{P}_{\eta} | \eta \rangle = i\partial/\partial_{\eta} | \eta \rangle$ $\left[\hat{Q}_{\eta}, \hat{P}_{\eta} \right] = i\hat{S}$

These canonical collective operators in S can be easily expressed in terms of the microscopic degrees of freedom⁽⁶⁾. We can also express any operator defined in S in terms of \hat{Q}_{η} and \hat{P}_{η} . For example, the GCM collective hamiltonian is given by⁽⁹⁾

$$H_{C}^{GCM} = \sum_{m=0}^{\infty} \frac{1}{2^{m}} : \hat{P}_{\eta}^{m} \hat{H}^{(m)} (\hat{Q}_{\eta}) : \qquad \text{II.8}$$

In eq. II.8 the normal order is defined as

$$: \widehat{P}_{\eta}^{m} \widehat{H}^{(m)} (\widehat{Q}_{\eta}) := \sum_{k=0}^{\infty} C_{k}^{m} \widehat{P}_{\eta}^{k} \widehat{H}^{(m)} (\widehat{Q}_{\eta}) \widehat{P}_{\eta}^{m-k}$$
$$= \{ \widehat{P}_{\eta}, \{ \widehat{P}_{\eta} \dots \{ \widehat{P}_{\eta}, \widehat{H}(\widehat{Q}_{\eta}) \} \dots \} \}$$

m anti-commutators

and

$$\widehat{H}^{(m)}(\widehat{\eta}) = \int d\xi \frac{(-i\xi)^m}{m!} < \eta + \xi/2 |\widehat{H}| \eta - \xi/2 >$$

$$= \int d\xi \frac{(-i)^{m}}{m!} < \eta + \xi/2 \left[\hat{Q}_{\eta}, \left[\hat{Q}_{\eta}, \dots \left[\hat{Q}_{\eta}, \hat{H} \right] \dots \right] \right] |\eta - \xi/2 > m - commutators$$

This shows that we can always write the dynamical equation II.1 in the form a Schroedinger type equation in the coordinate representation $|\eta>$. However, in general, this Schroedinger type equation has a "velocity"-dependent potential and a "mass-parameter", which depends on the coordinate.

III - SPECIAL CASES AND EXAMPLES

III-1 - TRANSLATIONAL INVARIANT OVERLAP KERNELS (6)

Translational invariant overlap kernels depend only on the difference of the generator coordinates whether the dependence of the generator coordinates whether the dependence of the dependence

$$\int \langle \alpha | \alpha' \rangle u_{k}(\alpha') d\alpha' = 2\pi \Lambda(k) u_{k}(\alpha)$$

where

$$u_k(\alpha) = \frac{1}{\sqrt{2\pi}} e^{ik\alpha_k - i\beta_k \alpha_k}$$
 (111.3)

$$\Lambda(\mathbf{k}) = \frac{1}{2\pi} \int \mathbf{N}(\alpha) e^{-i\mathbf{k}\alpha} d\alpha \qquad \text{III.4}$$

In this case the "coordinate" representation is the Fourier transform of the "momentum" representation

7

$$|x\rangle = \frac{1}{\sqrt{2\pi}} \int |k\rangle e^{-ikx} dk$$

and the pair of canonical collective variables defined as

$$\hat{Q}_{S} | x > = x | x >$$

 $\hat{P}_{S} | x > = i \partial_{x} | x >$
III.6

satisfy the eqs.

$$\hat{Q}_{\mathbf{S}} | \mathbf{k} \rangle = -\mathbf{i} \partial_{\mathbf{k}} | \mathbf{k} \rangle$$
 is the state we denote the set of the set of the state of

The gaussian overlap kernel is a special case of a translational invariant overlap kernel where

$$<\alpha \mid \alpha' > = e^{-(\alpha - \alpha')^2 / 4b_0^2}$$

$$\Lambda(\mathbf{k}) = \frac{b_0}{\sqrt{\pi}} e^{-\mathbf{k}^2 b_0^2}$$
III.8
III.8

Until now we considered only the continuous "coordinate" or "momentum" representations. We could also have considered discrete representations which diagonalize a boson number operator constructed in terms of \hat{Q}_{S} and \hat{P}_{S} . Taking the case of a Gaussian overlap kernel as an example and expanding the reduced energy kernel, $h(\alpha, \alpha')$

$$h(\alpha, \alpha') = \frac{\langle \alpha | H | \alpha' \rangle}{\langle \alpha | \alpha' \rangle},$$

in a power series in the generator coordinate one has,

$$h(\alpha,\alpha') = \sum_{n,m} \frac{h_{n,m}}{n!m!} (\alpha)^n (\alpha')^m$$

Introducing the boson operators

$$\hat{c} = \frac{1}{\sqrt{2}} \left(\frac{\hat{Q}_s}{b_o} + i\hat{P}_s b_o \right), \quad \left[\hat{c}, \hat{c}^+ \right] = \hat{s}$$

and using the expression of the GCM collective hamiltonian in the "coordinate" representation (see eq. II.4), one can easily show that ⁽⁸⁾

8

Therefore, the expansion of the reduced energy kernel in the generator coordinate is equivalent to a boson expansion of the collective hamiltonian, where the boson is constructed in terms of the collective canonical operators in S, \hat{Q}_{S} and \hat{P}_{S} .

 $\hat{H}_{C}^{GCM} = \sum_{n,m} \frac{h_{n,m}}{n!m!} (\sqrt{2} b_{0})^{n+m} (\hat{C}^{+})^{m} (\hat{C})^{n}$

In order to shed light on the origin of the singular behaviour of the weight function consider again the case of a Gaussian overlap and a quadratic approximation to the reduced energy kernel.

$$h(\alpha, \alpha') = h_0 + \frac{1}{2} \left[h_{20}(\alpha^2 + \alpha'^2) + 2h_{11}\alpha\alpha' \right] + \dots$$
 III.9

The collective hamiltonian \hat{H}_{C}^{GCM} can be written in this case as,

$$\hat{H}_{C}^{GCM} = E_{O} + \frac{\hat{P}_{S}^{2}}{2M} + \frac{1}{2} K_{M}^{2} \hat{Q}_{S}^{2} - E_{PZ}^{2}$$
 III.10

where the zero point energy E_{PZ} , the mass parameter M and the spring constant K_M are respectively given by

$$E_{pZ} = b_{0}^{2} h_{11}$$

$$M^{-1} = 2(h_{11} - h_{20})b_{0}^{4}$$
III.11
$$K_{M} = 2(h_{11} + h_{20})$$

The hamiltonian III.10 is a standard harmonic oscillator hamiltonian and its eigenfunctions are harmonic oscillator wave functions $\phi_n^{ho}(x/b_c)$ and its eigenvalues referred to the unperturbed ground state are

$$E_n = \hbar \omega_c (n+1/2) - E_{PZ}$$

where

$$\hbar\omega_{c} = 2b_{0}^{2}\sqrt{(h_{11}^{2} - h_{20}^{2})}$$

$$b_{c}^{2} = \sqrt{\frac{h_{11}^{-h_{20}}}{h_{11}^{+h_{20}}}} \quad b_{0}^{2}$$

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9

To proceed, consider the ground state wave function

$$\phi_{0}(x/b_{c}) = \frac{1}{\sqrt{b_{c}}\sqrt{\pi}} e^{-x^{2}/2b_{c}^{2}}$$
 III.12

even and The weight function associated to this state is a (see eq. bd. 1.8). A second of the market of an even of the sub- second sectors (from (proceeded))

$$\mathbf{f}(\alpha) = \sqrt{\mathbf{b}_{c}}/\mathbf{b}_{0} \qquad \int d\mathbf{k} \frac{\mathbf{e}^{\mathbf{i}\mathbf{k}\alpha}}{2^{\pi}} \frac{\mathbf{e}^{\mathbf{k}^{2}}(\mathbf{b}_{c}^{2}-\mathbf{b}_{0}^{2})/2}{2^{\pi}}$$

which exists as a regular function as long as $b_c^2 > b_0^2$. The nature of this singular behaviour is equivalent to the high-momentum divergence considered in ref. 10 and it stems from the fact that when $b_c < b_0$, a function which has high "momentum" components is being expanded in terms of a wave-packet which has only "low" momentum components ⁽⁶⁾. Indeed, the wave functions associated by the "momentum" representation to the groundstate and to the generator state are respectively,

and

$$\langle \mathbf{k} | \phi_{\mathbf{o}} \rangle = \sqrt{\frac{\mathbf{c}}{\sqrt{\pi}}} \mathbf{e}^{\mathbf{c}} \mathbf{c}^{\mathbf{c}}$$

 \sqrt{b}

$$k \mid \alpha > = e^{-ik\alpha} \sqrt{\frac{b}{\sqrt{\pi}}} e^{-k^2 b_0^2/2}$$

 $-b^{2}k^{2}/2$

which shows the correctness of our statement

III-2 ONE AND TWO-CONJUGATE PARAMETER FAMILIES OF GENERATOR STATES (9)

states (OPF and TCPF) are defined respectively as the state (option of the states (optio

$$|\alpha\rangle = e^{-i\alpha P} |0\rangle$$
$$|\alpha,\beta\rangle = e^{-i\alpha \hat{P}} e^{i\beta \hat{Q}} |0\rangle$$

where Q and P are canonical operators in the many-body Hilbert space

$$\left[\hat{Q},\hat{P}\right] = i$$

The overlap kernel of the OPF is a translational invariant

overlap kernel and so it can be diagonalized by a Fourier transformation

$$\int \langle \alpha | \alpha' \rangle u_{k}(\alpha') d\alpha' = 2\pi \Lambda(k) u_{k}(\alpha)$$

where

 $\mathbf{u}_{\mathbf{k}}(\alpha) = \frac{e^{\mathbf{i}\mathbf{k}\alpha}}{\sqrt{2\pi}}$

and

$$\Lambda(\mathbf{k}) \stackrel{\text{\tiny def}}{=} < 0 \stackrel{\text{\tiny def}}{=} \frac{\mathbf{\widehat{n}} \mathbf{\widehat{p}} \mathbf{\widehat{y}}}{\mathbf{k}} \quad | 0 > \qquad \text{\tiny def} \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix} \stackrel{\text{\tiny def}}{=} \begin{bmatrix} 0 \\ 0 \end{bmatrix} \right) \stackrel{\text{\tiny def}}{=} \frac{\mathbf{\widehat{n}} \mathbf{\widehat{n}} \mathbf{\widehat{p}}}{\mathbf{k}}$$

 \widehat{II}_k^{PY} is the Peierls-Yoccoz projection operator associated with the operator \widehat{P}

$$\hat{\mathbf{I}}_{\mathbf{k}}^{\mathbf{PY}} = \frac{1}{2\pi} \int e^{\mathbf{i}\mathbf{k}\alpha} e^{-\mathbf{i}\alpha\hat{\mathbf{P}}} d\alpha$$

$$= \delta(\hat{\mathbf{P}} - \mathbf{k})$$

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III.16

Thus, the standard orthonormal "momentum" representation in the GCM collective subspace S, associated with the OPF of generator states is identical to the normalized Peierls-Yoccoz projection of the reference state |0>, associated with the operator \hat{P} $|\psi_k\rangle_Y = \frac{\hat{\pi}_k^{PY} |0\rangle}{\sqrt{\langle 0 | \hat{\pi}_k^{PY} | 0 \rangle}}$ III.15

By construction one has

$$\hat{\mathbf{P}} | \psi_{\mathbf{k}} \rangle_{\mathbf{Y}} = \mathbf{k} | \psi_{\mathbf{k}} \rangle_{\mathbf{Y}}$$

and the pair of canonical collective operators in Signare given by 200 and

$$\hat{\mathbf{p}}_{s_1} = \hat{\mathbf{s}}_1 \hat{\mathbf{p}} = \hat{\mathbf{p}} \hat{\mathbf{s}}_1$$
$$\hat{\mathbf{q}}_{s_1} = \hat{\mathbf{s}}_1 \hat{\mathbf{q}} \hat{\mathbf{s}}_1$$

However, in general

$$\left[\hat{Q},\hat{S}_{1}\right] \neq 0$$

so \hat{S}_1 is not an eigenspace of \hat{Q} and we cannot find a base in S_1 which

diagonalizes Q.

On the other hand, the overlap kernel for the TCPF is

$$\langle \alpha\beta | \alpha'\beta' \rangle = \langle 0 | e^{-i\beta\hat{Q}} e^{i\alpha\hat{P}} e^{-i\alpha'\hat{P}} e^{i\beta'\hat{Q}} | 0 \rangle$$

and its eigenfunctions and eigenvalues are determined by the equation

$$\int \langle \alpha\beta | \alpha'\beta' \rangle \phi_{n;k}(\alpha',\beta') d\alpha' d\beta' = 2 \pi \lambda_n(k) \phi_{n;k}(\alpha,\beta).$$

It can be easily shown that $\phi_{n;k}(\alpha,\beta)$ is given by ⁽⁹⁾

$$\phi_{n;k}(\alpha,\beta) = \frac{e^{ik\alpha}}{\sqrt{2\pi}} \phi_n(\beta-k)$$

and the $\lambda_n(\mathbf{k})$ are independent of k.

The functions $\phi_n(\beta)$ and the λ_n are eigenfunctions and eigenvalues of the semi-positive definite Hilbert-Schmidt overlap kernel $\tilde{N}(\beta,\beta')$

$$\tilde{N}(\beta,\beta') = \langle 0 | e^{-i\beta \tilde{Q}} \delta(\hat{P}) e^{i\beta' \tilde{Q}} | 0 \rangle$$

The Hilbert-Schmidt kernel III.17 can have zero eigenvalues and when they occur there are two-important consequences. One is that the weight functions defined in the null space of \tilde{N} gives rise to vectors of zero norm in the many-body H.S. Therefore there is no loss of generality if we restrict the weight function space to the orthogonal complement of the null space of \tilde{N} . The other is that the existence of eigenvectors of \tilde{N} with zero eigenvalues implies that the generator states are not linearly independent.

In this case the standard orthonormal representation in the GCM collective subspace S_2 associated with the TCPF of generator states is given by the Peierls-Thouless projection of the reference state $|0\rangle$ associated with the operator \hat{P}

$$|\psi_{\mathbf{k};\mathbf{n}}\rangle_{\mathbf{T}} = \frac{\overline{\Pi_{\mathbf{k},\mathbf{n}}}^{\mathbf{PT}} |0\rangle}{\sqrt{\lambda_{\mathbf{n}}}}, \quad \lambda_{\mathbf{n}} \neq 0$$

In eq. III.18 $\hat{\mathbb{I}}_{k,n}^{PT}$ is the so-called Peierls-Thouless double projection operator

$$\hat{I}_{k,n}^{PT} = \int d\alpha d\beta \, \frac{e^{ik\alpha}}{2\pi} \, \phi_n(\beta-k) \, e^{i\alpha \hat{P}} \, e^{i\beta \hat{Q}}$$

III.18

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III.l

By construction one has founded the second second of Antonian and for rescaled of the second of the second of the second second second of the second secon

$$\mathbf{P}[\boldsymbol{\psi}_{k,n}, \mathbf{T}] \stackrel{\text{def}}{=} \mathbf{k}[\boldsymbol{\psi}_{k,n}, \mathbf{T}] \quad \text{if} \mathbf{III}.19$$

and it can be easely shown that (9)

$$\hat{Q}|\psi_{k,n}\rangle_{T} = -i\partial_{k}|\psi_{k,n}\rangle_{T}$$
III.20

Therefore the pair of canonical collective operators associated with the continuous label k are in this case given by

$$\hat{\mathbf{P}}_{\mathbf{S}_{2}} = \hat{\mathbf{S}}_{2}\hat{\mathbf{P}} = \hat{\mathbf{P}}\hat{\mathbf{S}}_{2} \quad \text{def}\left[\frac{2}{2}\hat{\mathbf{Q}}_{\mathbf{S}_{2}}\hat{\mathbf{S}}_{\mathbf{S}_{2}} + \frac{1}{2}\hat{\mathbf{S}}_{\mathbf{S}_{2}}\hat{\mathbf{S}}_{\mathbf{S}_{2}} + \frac{1}{2}\hat{\mathbf{S}}_{\mathbf{S}_{2}}\hat{\mathbf{S}}_{\mathbf{S}_{2}} + \frac{1}{2}\hat{\mathbf{S}}_{\mathbf{S}_{2}}\hat{\mathbf{S}}_{\mathbf{S}_{2}} + \frac{1}{2}\hat{\mathbf{S}}_{\mathbf{S}_{2}}\hat{\mathbf{S}}_{\mathbf{S}_{2}} + \frac{1}{2}\hat{\mathbf{S}}_{\mathbf{S}_{2}}\hat{\mathbf{S}}_{\mathbf{S}_{2}} + \frac{1}{2}\hat{\mathbf{S}}_{\mathbf{S}_{2}}\hat{\mathbf{S}}_{\mathbf{S}_{2}} + \frac{1}{2}\hat{\mathbf{S}}_{\mathbf{S}_{2}}\hat{\mathbf{S}}_{\mathbf{S}_{2}}\hat{\mathbf{S}}_{\mathbf{S}_{2}} + \frac{1}{2}\hat{\mathbf{S}}_{\mathbf{S}_{2}}\hat{\mathbf{S}}_{\mathbf{S}_{2}}\hat{\mathbf{S}}_{\mathbf{S}_{2}} + \frac{1}{2}\hat{\mathbf{S}}_{\mathbf{S}_{2}}\hat{\mathbf$$

Thus in the TCPF case S_2 is an eigenspace of both Q and P and by an unitary transformation we can find a basis which diagonalizes \hat{Q} . This basis is the Fourier transform of the states $|\psi_{k,n}\rangle_{T}$ and it is given by the Peierls-Thouless projection of the reference state $|0\rangle$ associated with the operator \hat{Q} ,

$$\psi_{\mathbf{x},\mathbf{n}} >_{\mathbf{T}} = \frac{\widehat{\Pi}_{\mathbf{x},\mathbf{n}}^{\mathbf{PT}} |0\rangle}{\sqrt{\lambda_{\mathbf{n}}}}, \quad \lambda_{\mathbf{n}} \neq 0$$

III.22

 $= \frac{1}{2\pi} \int |\psi_{\mathbf{k},\mathbf{n}}|^2 e^{-\mathbf{i}\mathbf{k}\cdot\mathbf{x}} d\mathbf{k}$

To proceed in the discussion about the physical properties of the GCM collective subspaces, one introduce a canonical transformation from the microscopic degrees of freedom to collective, \hat{Q} and \hat{P} , and intrinsic degrees of freedom. Together with \hat{Q} and the remaining N-1 intrinsic operators $\hat{\xi}_1, \hat{\xi}_2, \dots, \hat{\xi}_{N-1}$, which by the canonical nature of the transformation must commute with both \hat{Q} and \hat{P} , we can arrive at a coordinate representation of the full many-body H.S. defined by the kets $|Q,\xi\rangle$ chosen as eigenkets of \hat{Q} and $\hat{\xi}$. This representation is a product representation and the states $|Q\rangle$ span a H.S. of one single degree of freedom, the collective space and the $|\xi\rangle$ are likewise associated with a H.S. of N-1 degrees of freedom, the intrinsic space. However it should always be kept in mind that both S_1 and S_2 carry all the N degrees of freedom of the many-body system under consideration. They are distinguished from the full many-body H.S. in that

they contain various imposed correlations among the N degrees of freedom. The discussion which follows will be aimed precisely at exhibiting the general nature of these correlations in each of the two cases.

We begin by considering the wave function associated to the states $|\psi_{k;n}\rangle_T$ by the $|Q,\xi\rangle$ representation ,

$$\langle Q\xi | \psi_{k;n} \rangle_{T} = \frac{e^{ikQ}}{\sqrt{2\pi}} X_{n}(\xi)$$

where

$$X_{n}(\xi) = \frac{1}{\sqrt{\lambda n}} \int \phi_{n}(Q) < Q\xi \mid 0 > dQ$$

and $\phi_n(Q)$ is the Fourier transform of $\phi_n(\beta)$.

The states $X_n(\xi)$ are orthonormal and depend only on the intrinsic variables and so $|\psi_{k,n}\rangle_T$ comes out as a product of a collective wave function and an intrinsic wave function, and this holds even when $|0\rangle$ is not itself a product wave function. Indeed, the wave function associated to the reference state $|0\rangle$ by the $|Q,\xi\rangle$ representation can be shown to be given by (9)

 $\langle Q\xi | 0 \rangle = \sum_{n,\lambda_n \neq 0} \sqrt{\lambda_n} \phi_n(Q) X_n(\xi)$

Thus we see that the reference state $|0\rangle$ is given by a sum of products of collective and intrinsic states, the number of terms in the sum being equal to the number of eigenvectors of $\tilde{N}(\beta,\beta')$ with eigenvalue different from zero.

In the case of the OPF,the wave function associated to the states $|\psi_k\rangle_{\rm Y}$ by the $|Q,\xi\rangle$ representation are $^{(9)}$

$$\frac{\partial \left[\left(\left\{ x \right\} \right] + \left\{ x \right\} \right]}{\sqrt{2\pi}} = e^{\frac{1}{2} \frac{\mathbf{e}^{-\mathbf{i} \mathbf{k} \mathbf{Q}}}{\sqrt{2\pi}}} \cdot \left\{ \mathbf{x}_{\mathbf{k}}^{-}(\boldsymbol{\xi}) \right\} = e^{\frac{1}{2} \frac{\mathbf{e}^{-\mathbf{i} \mathbf{k} \mathbf{Q}}}{\sqrt{2\pi}}} \cdot \left\{ \mathbf{x}_{\mathbf{k}}^{-}(\boldsymbol{\xi}) \right\}$$

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$$X_{k}(\xi) = \frac{1}{\sqrt{\sum_{n,\lambda_{n}\neq 0} \lambda_{n} |\phi_{n}(k)|^{2}}} \sum_{n,\lambda_{n}\neq 0} \sqrt{\lambda_{n}} \phi_{n}(k) X_{n}(\xi)$$

Therefore the states $|\psi_k\rangle_{Y}$ are given by the product of a collective wave function and an intrinsic wave function. However, the intrinsic wave function depends on the eigenvalue k of the operator \hat{P} . This property is responsable for the fact that \hat{S}_1 is not an eigenspace of \hat{Q} .

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On the other hand if the reference state itself is a product wave function

$$= \phi_{0}(Q) X_{0}(\xi)$$
,

in which case N has only one eigenvector with eigenvalue different from zero, one has

$$\mathbf{X}_{\mathbf{k}}^{c}(\boldsymbol{\xi}) = \mathbf{X}_{\mathbf{0}}(\boldsymbol{\xi})^{c}$$
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 $|\psi_{k,0}\rangle_T$ becomes equal to $|\psi_k\rangle_Y$ and the subspaces S_1 and S_2 becomes identical. If we identify the canonical operators \hat{Q} and \hat{P} with the center of mass coordinate and momentum respectively, the above discussions shows that in general the subspace associated with the OPF of generator states is not galilean invariant. It is galilean invariant only when the reference state itself is a product wave function. This fact is responsable for the incorrect translational mass that one in general obtains in GCM with generator states chosen as in eq. III.13. On the other hand, the subspace associated with the TCPF is always a galilean invariant subspace and this is true even in the case when the reference state is not itself a product wave function. However when the reference state admits itself a factorization into a product of collective and intrinsic wave-functions both spaces are galilean invariant and identical.

To conclude, in general the TCPF which depends on twogenerator coordinates describes two-degrees of freedom, one collective and other non-collective (it depends only on the intrinsic degrees of freedom), and its nature depends only on the correlations imposed on the reference state $|0\rangle$. When we make this identification we are supposing that the dynamical variables which are diagonal in the basis obtained by the diagonalization of the overlap kernel are the appropriate ones (if not, they can be found by unitary transformations in S).

Furthermore the GCM collective subspace has the property that those two degrees of freedom are kinematically decoupled. They are coupled by the dynamics, in other words by the GCM collective hamiltonian, which can be easily written down in terms of these two degrees of freedom fullowing ref. 9. However we are in general interested in cases when the coupling of the collective and non-collective degrees of freedom is small so that one has almost decoupled bands. In that case we can always restrict the non-collective degree of freedom to be in the lowest energy state and so the dynamics reduces to the collective dynamics only⁽¹¹⁾. On the other hand when the generator states are so redundant that there is only one eigenvector of \tilde{N}

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with non-zero eigenvalue the TCPF which depends on two parameters describes only one degree of freedom, the collective one. In this case the TCPF is redundant in the sense that the collective subspace associated with the one and two conjugate parameter family of generator states are identical⁽¹¹⁾. This happens when the reference state itself factorizes into a product of a collective wave function and an intrinsic wave function. However in the case when the reference state does not admit this factorization, the two subspaces are different and the collective and non-collective degrees of freedom are knematically coupled in the GCM collective subspace æsociated with the OPF of generator states.

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